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Access DB#	. ,	-		

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: RIP #		Examiner #: 78680 Date: 1EB 26, 2003			
Art Unit: 1713 Phone N	lumber 30 6-0094	Serial Number: 10/04-9, 861			
Mail Box and Bldg/Room Location	: <u>CP3 8C32</u> Resu	Ilts Format Preferred (circle): PAPER DISK E-MAIL			
Manage About and a second to see	*** • • • • • • • • • • • • • • • • • •				
If more than one search is subm	ittea, piease prioritiz *******	e searches in order of need. ***********************************			
Please provide a detailed statement of the	search topic, and describe a	as specifically as possible the subject matter to be searched.			
Include the elected species or structures, ke	eywords, synonyms, acron	yms, and registry numbers, and combine with the concept or			
utility of the invention. Define any terms	that may have a special me	aning. Give examples or relevant citations, authors, etc, if			
known. Please attach a copy of the cover s	neet, pertinent claims, and	abstract.			
Title of Invention: BISIMIDINO compounds and transition metal complexes thereof					
Inventors (please provide full names):	KILDSTEIN, Ben	10; GONZOUKH, Andrei; KRISTEN, Marc			
N	3/				
Earliest Priority Filing Date: Aug 20 1999					
*For Sequence Searches Only * Please includ	le all pertinent information (p	parent, child, divisional, or issued patent numbers) along with the			
appropriate serial number					
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Please search for metal con	speres comaining	the following diimine fragments			
(cf. Claims 1 and 9)	•				
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STAFF USE ONLY	Type of Search	Vendors and cost where applicable			
Searcher: _ Calle	NA Sequence (#)	STN			
Searcher Phone #:	AA Sequence (#2	Dialog			
Searcher Location:	Structure (#)	Questel/Orbit			
Date Searcher Picked Up: 3 5 03	Bibliographic	Dr. Link			
Date Completed: 3603	Litigation	Lexis/Nexis			
Searcher Prep & Review Time:	Fulltext	Sequence Systems			
Clerical Prep Time:	Patent Family	WWW/Internet			
Online Time:	Other	Other (specify)			

PTO-1590 (8-01)

=> file reg

'RIP,

I did one parent structure and two subset structures. In L15 (the first substructure search printed) I specified that the nitogen in R1, in claim 1 - "NR5R6" - is a ring system.

From these results I did a search for a both metals then specifically for transition metals. The metals are printed out first in this printout (L20/L31).

The other substructure search I performed was to specify R3 as H, Carbocyclic or alkyl. I was getting many answers where the C bonded to R3 was a carbonyl group. Those answers are printed out L32 after the metals.

Lastly the the balance were printed out (L36 1-25).

If you have any questions please feel free to call me at your convenience.

John

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

4 MAR 2003 HIGHEST RN 496907-99-4 STRUCTURE FILE UPDATES: 4 MAR 2003 HIGHEST RN 496907-99-4 DICTIONARY FILE UPDATES:

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

=> d his

(FILE 'HOME' ENTERED AT 08:24:56 ON 06 MAR 2003)

FILE 'LREGISTRY' ENTERED AT 08:25:12 ON 06 MAR 2003 ACTIVATE RIPLEE/L

L1

STR

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ACTIVATE RIPLEEL1/L
L2
               STR
               STR L1
L3
               STR L2
L4
     FILE 'REGISTRY' ENTERED AT 08:36:22 ON 06 MAR 2003
           11 S L4
L5
     FILE 'LREGISTRY' ENTERED AT 08:36:37 ON 06 MAR 2003
L6
               STR L1
     FILE 'REGISTRY' ENTERED AT 08:51:10 ON 06 MAR 2003
L7
            11 S L6
     FILE 'LREGISTRY' ENTERED AT 08:52:12 ON 06 MAR 2003
L8
               STR L6
     FILE 'REGISTRY' ENTERED AT 09:04:53 ON 06 MAR 2003
L9
             0 S L8
     FILE 'LREGISTRY' ENTERED AT 09:05:28 ON 06 MAR 2003
     FILE 'REGISTRY' ENTERED AT 09:07:13 ON 06 MAR 2003
L10
            11 S L6
           2242 S L6 FULL
L11
                SAVE L11 RLEE143/A
     FILE 'HCA' ENTERED AT 09:08:15 ON 06 MAR 2003
           699 S L11
L12
     FILE 'REGISTRY' ENTERED AT 09:08:28 ON 06 MAR 2003
L13
               STR L6
             9 S L13 SSS SAM SUB=L11
L14
            155 S L13 SSS FULL SUB=L11
L15
               SAVE RLEE143A/A L15
             58 S L15 AND 1-5/M
L16
             46 S L15 AND (T1 OR T2 OR T3)/PG
L17
     FILE 'HCA' ENTERED AT 09:12:01 ON 06 MAR 2003
             43 S L15
L18
             12 S L16
L19
            11 S L17
L20
     FILE 'LREGISTRY' ENTERED AT 09:12:46 ON 06 MAR 2003
L21
                STR L6
L22
                STR L21
                STR L22
L23
     FILE 'REGISTRY' ENTERED AT 09:22:56 ON 06 MAR 2003
L24
             50 S L22 SSS SAM SUB=L11
              6 S L23 SSS SAM SUB=L11
L25
     FILE 'LREGISTRY' ENTERED AT 09:23:50 ON 06 MAR 2003
L26
               STR L23
     FILE 'REGISTRY' ENTERED AT 09:30:08 ON 06 MAR 2003
              3 S L26 SSS SAM SUB=L11
L27
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L28 81 S L26 SSS FULL SUB=L11 SAVE L28 RLEE861B/A

L29 38 S L28 NOT L17

FILE 'HCA' ENTERED AT 09:32:12 ON 06 MAR 2003

L30 12 S L29

FILE 'REGISTRY' ENTERED AT 09:36:18 ON 06 MAR 2003

L33 37 S L28 NOT L16

FILE 'HCA' ENTERED AT 09:36:48 ON 06 MAR 2003

L34 11 S L33

L35 17 S L34 OR L20

L36 25 S L18 NOT (L19 OR L32)

FILE 'REGISTRY' ENTERED AT 09:38:47 ON 06 MAR 2003

=> d que stat L15

L6 STR

REP G1 = (1-2) C

VAR G2=N/S/O/P

NODE ATTRIBUTES:

NSPEC IS RC AT 11
NSPEC IS RC AT 15
DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L11 2242 SEA FILE=REGISTRY SSS FUL L6

L13 STR

REP G1=(1-2) C
VAR G2=N/S/O/P
NODE ATTRIBUTES:
NSPEC IS RC AT 11
NSPEC IS R AT 15
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L15 155 SEA FILE=REGISTRY SUB=L11 SSS FUL L13

100.0% PROCESSED 2242 ITERATIONS 155 ANSWERS

SEARCH TIME: 00.00.01

REP G1=(1-2) C
VAR G2=N/S/O/P
NODE ATTRIBUTES:
NSPEC IS RC AT 11
NSPEC IS RC AT 15
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 10 STEREO ATTRIBUTES: NONE

2242 SEA FILE=REGISTRY SSS FUL L6 L11 L26 STR

C√Ak

@17 18

C~ Cb

@20 21

10 N Ν

REP G1 = (1-2) C VAR G2=N/S/O/P VAR G3=CH/17/20 NODE ATTRIBUTES:

NSPEC IS RC 15 AΤ IS R AT 16 NSPEC DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

81 SEA FILE=REGISTRY SUB=L11 SSS FUL L26 L28

1433 ITERATIONS 100.0% PROCESSED

81 ANSWERS

SEARCH TIME: 00.00.01

=> file hca FILE 'HCA' ENTERED AT 09:40:00 ON 06 MAR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 27 Feb 2003 VOL 138 ISS 10 FILE LAST UPDATED: 27 Feb 2003 (20030227/ED)

This file contains CAS Registry Numbers for easy and accurate

substance identification.

Rip. this record should have a non-=> d L31 1 cbib abs hitstr

trainsition me L31 ANSWER 1 OF 1 HCA COPYRIGHT 2003 ACS 113:40323 Preparation of 3-acylamino-1-[[(heterocyclylsulfonyl)amino]carbonyl]-2-azetidinones as antibiotics. Treuner, Uwe D. (Squibb, E. R., and Sons, Inc., USA). Eur. Pat. Appl. EP 336369 A1 19891011, 69 pp. DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1989-105883 19890404. PRIORITY: US 1988-177207 19880404.

OCH2Ph

ΙI

GI

$$R^{1}NH \longrightarrow R^{3}$$
 R^{2}
 R^{3}
 R^{2}
 R^{3}
 R^{3}
 R^{2}
 R^{3}
 R^{3}
 R^{2}
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 $R^$

OCH2Ph PhCH2O2CNH NNHCO NCONHSO2N

NOCMe2CO2H OH CONH NCONHSO2N NNHCO III

The title compds. [I; R = [(oxopyridinylcarbonyl)amino]oxoimidazolo, AB -dioxopiperazino, etc.; R1 = acyl; R2, R3 = H, alkyl, alkenyl, etc.] were prepd. as antibiotics (no data). Thus, I.CF3CO2H [R = [(tert-butoxycarbonyl)amino]oxoimidazolo] (prepn. given) was treated with CF3CONMeSiMe3 and the product condensed with 1H-benzotriazol-1-yl 6-difluoromethyl-4,5-bis(phenylmethoxy)-2-pyridinecarboxylate (prepn. given) to give, after neutralization, title compd. II. Na which was converted in 2 steps to title compd. (3S)-(Z)-III.2Na.

127324-29-2P 127324-30-5P 127324-34-9P IΤ

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in prepn. of antibiotics)

RN 127324-29-2 HCA

Carbamic acid, [1-[[[[3-[[[(1,1-dimethylethoxy)carbonyl]amino]methyl]-CN 4,5-bis(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-2-oxo-1imidazolidinyl]sulfonyl]amino]carbonyl]-2-oxo-3-azetidinyl]-, phenylmethyl

ester, monosodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

$$t-BuO-C-NH-CH_2$$
 $O-CH_2-Ph$
 $O-CH_2-Ph$

■ N =

RN 127324-30-5 HCA

CN Carbamic acid, [1-[[[[3-[[[6-[[(aminocarbonyl)amino]methyl]-4,5-bis(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-2-oxo-1-imidazolidinyl]sulfonyl]amino]carbonyl]-2-oxo-3-azetidinyl]-, phenylmethyl ester, monosodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

$$H_2N-C-NH-CH_2$$
 $O-CH_2-Ph$
 $O-CH_2-Ph$

Na

RN 127324-34-9 HCA

CN Carbamic acid, [1-[[[[3-[[[6-(aminocarbonyl)-4,5-bis(phenylmethoxy)-2-pyridinyl]carbonyl]amino]-2-oxo-1-imidazolidinyl]sulfonyl]amino]carbonyl]-2-oxo-3-azetidinyl]-, phenylmethyl ester, monosodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

$$H_2N-C$$
 $O-CH_2-Ph$
 $O-CH_2-Ph$

Na

127324-28-1P 127324-35-0P 127324-38-3P ΙT

127337-92-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of, as antibiotic)

RN

127324-28-1 HCA
Pyridinium, 1-[[6-[[[3-[[[3-[[(2-amino-4-thiazolyl)[(1-carboxy-1-CN methylethoxy)imino]acetyl]amino]-2-oxo-1-azetidinyl]carbonyl]amino]sulfony 1]-2-oxo-1-imidazolidinyl]amino]carbonyl]-1,4-dihydro-3-hydroxy-4-oxo-2pyridinyl]methyl]-, inner salt, monosodium salt, [S-(Z)]- (9CI) (CA INDEX NAME)

0

PAGE 1-A

Na

PAGE 1-B

RN 127324-35-0 HCA

CN Propanoic acid, 2-[[[1-(2-amino-4-thiazolyl)-2-[[1-[[[[3-[[[6-(aminocarbonyl)-1,4-dihydro-5-hydroxy-4-oxo-2-pyridinyl]carbonyl]amino]-2-oxo-1-imidazolidinyl]sulfonyl]amino]carbonyl]-2-oxoethylidene]amino]oxy]-2-methyl-, diphenylmethyl ester, disodium salt, [S-(Z)]- (9CI) (CA INDEX NAME)

•2 Na

RN 127324-38-3 HCA

CN Propanoic acid, 2-[[[1-(2-amino-4-thiazolyl)-2-[[1-[[[[3-[[(6-cyano-1,4-dihydro-5-hydroxy-4-oxo-2-pyridinyl)carbonyl]amino]-2-oxo-1-imidazolidinyl]sulfonyl]amino]carbonyl]-2-oxo-3-azetidinyl]amino]-2-

oxoethylidene]amino]oxy]-2-methyl-, disodium salt, [S-(Z)]-(9CI) (CA INDEX NAME)

●2 Na

RN 127337-92-2 HCA

CN Propanoic acid, 2-[[[2-[[1-[[[[3-[[[6-[[(aminocarbonyl)amino]methyl]-1,4-dihydro-5-hydroxy-4-oxo-2-pyridinyl]carbonyl]amino]-2-oxo-1-imidazolidinyl]sulfonyl]amino]carbonyl]-2-oxo-3-azetidinyl]amino]-1-(2-amino-4-thiazolyl)-2-oxoethylidene]amino]oxy]-2-methyl-, disodium salt (9CI) (CA INDEX NAME)

PAGE 1-A

Me

HO2C-C-O-N

Me O

NH-C-C

2 Na

PAGE 1-B

=> d L20 1 cbib abs hitstr

Transition Metals

L20 ANSWER 1 OF 11 HCA COPYRIGHT 2003 ACS

137:370387 N-pyrrolyl-[N,N,N]-bis(imino)pyridyl iron(II) and cobalt(II) olefin polymerization catalysts. Amort, Christoph; Malaun, Michael; Krajete, Alexander; Kopacka, Holger; Wurst, Klaus; Christ, Maria; Lilge, Dieter; Kristen, Marc O.; Bildstein, Benno (Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Innsbruck, A-6020, Austria). Applied Organometallic Chemistry, 16(9), 506-516 (English) 2002. CODEN: AOCHEX. ISSN: 0268-2605. Publisher: John Wiley & Sons Ltd..

A series of new [N,N,N]-2,6-bis(imino)pyridyl iron and cobalt halide AΒ complexes as precatalysts for the homo- and co-polymn. of ethylene has been synthesized and evaluated for their catalytic performance. The novel key structural feature of these [N,N,N]MCl2 catalysts is their peripheral substitution with bulky N-heterocyclic groups, including substituted N-pyrrolyl, N-indolyl, N-carbazolyl, and N-triazolyl moieties. The synthesis starts with the corresponding N-amino-N-heterocycles, which were prepd. by a modified Paal-Knorr condensation of 1,4-diketones with mono-protected hydrazines, or by electrophilic amination of benzannelated azoles. Condensation with 2,6-diacetylpyridine or 2,5-diformylthiophene afforded 14 different terdentate ligands, and complex formation with iron(II), iron(III), cobalt(II) yielded 23 different precatalysts. A single crystal structure anal. of one representative showed that these paramagnetic complexes have a distorted trigonal bipyramidal structure with orthogonal sterically shielding N-azolyl groups. All the methylalumoxane-activated iron(II) and cobalt(II) complexes with N-pyrrolyl, N-indolyl, and N-carbazolyl substituents are highly active catalysts for the homo- and co-polymn. of ethylene, producing polymers with comparatively narrow mol. wt. distributions and with a wide range of mol. wts., dependent on the substitution pattern of the peripheral N-azolyl substituents. The obsd. microstructures of the polymers vary from very highly branched to mostly linear, giving access to oligomers and polymers with an unusual broad spectrum of macroscopic phys. properties.

289708-74-3P 289708-75-4P 289708-76-5P 289708-77-6P 289708-81-2P 289708-82-3P 289708-96-9P 328239-71-0P 328239-72-1P 328239-73-2P 328239-76-5P 328239-76-6P 328239-77-6P 328239-78-7P 328239-79-8P 328239-80-1P 475471-28-4P 475471-29-5P 475471-30-8P 475471-31-9P 475471-32-0P 475471-33-1P

RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation);
PREP (Preparation); USES (Uses)

(prepn. of N-pyrrolyl-[N,N,N]-bis(imino)pyridyl iron(II) and cobalt(II)

olefin polymn. catalysts)

RN 289708-74-3 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-75-4 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-76-5 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-77-6 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-81-2 HCA

Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX
NAME)

RN 289708-82-3 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-96-9 HCA

CN Iron, trichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-71-0 HCA

CN Iron, trichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-72-1 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-73-2 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-74-3 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(2-methylphenyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-75-4 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(2-methylphenyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)-(9CI) (CA INDEX NAME)

RN 328239-76-5 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-1H-indol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-77-6 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-1H-indol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-78-7 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[9H-carbazol-9-amine-.kappa.NN9]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-79-8 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[9H-carbazol-9-amine-.kappa.NN9]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-80-1 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[3,5-dimethyl-4H-1,2,4-triazol-4-amine-.kappa.NN4]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 475471-28-4 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 475471-29-5 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 475471-30-8 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[1H-indol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 475471-31-9 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[1H-indol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 475471-32-0 HCA

CN Iron, dichloro[N-[1-[6-[1-[(2,5-dimethyl-1H-pyrrol-1-yl)imino-.kappa.N]ethyl]-2-pyridinyl-.kappa.N]ethylidene]-9H-carbazol-9-amine-.kappa.NN9]-, (SP-5-41)- (9CI) (CA INDEX NAME)

RN 475471-33-1 HCA

CN Cobalt, dichloro[N,N'-[(2,5-thiophenediyl-.kappa.S)dimethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-21)- (9CI) (CA INDEX

NAME)

=> d L20 2-11 cbib abs hitstr

L20 ANSWER 2 OF 11 HCA COPYRIGHT 2003 ACS

136:295220 Process and catalyst for the co-oligomerization of ethylene and alpha.-olefins. De Boer, Eric Johannes Maria; Deuling, Hendrikus Hyacinthus; Van der Heijden, Harry; On, Quoc An; Van Oort, Aart Bartus; Van Zon, Arie (Shell Internationale Research Maatschappij B.V., Neth.). PCT Int. Appl. WO 2002028805 A2 20020411, 71 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-EP11392 20011001. PRIORITY: EP 2000-308728 20001003; EP 2001-306601 20010801.

AB A process for prodn. of higher linear .alpha.-olefins and/or alkyl-branched .alpha.-olefins comprises the co-oligomerization of one or more .alpha.-olefins with ethylene in the presence of a metal catalyst system employing one or more bis-aryliminepyridine MXa complexes and/or one or more [bis-aryliminepyridine MYp.Lb+] [NC-]q complexes (M = Fe, Co; X = halide; a = 2,3; Y = ligand; p + q = 2 or 3; L is a neutral Lewis donor; b = 0-2); and the process is carried out at an ethylene pressure of less than 2.5 MPa. Ethylene and 1-heptene were oligomerized using a catalyst system contg. 2-[1-(2,4,6-trimethylphenylimino)ethyl]-6-[1-(4-tert-butylphenylimino) ethyl] pyridine iron[II] chloride complex and MAO.

IT 409127-10-2P

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(process and catalyst for the co-oligomerization of ethylene and .alpha.-olefins) $\begin{tabular}{ll} \end{tabular} \label{table}$

RN 409127-10-2 HCA

CN Iron, dichloro[N-[1-[6-[1-[(2,4,6-trimethylphenyl)imino-.kappa.N]ethyl]-2-pyridinyl-.kappa.N]ethylidene]-1H-pyrrol-1-amine-.kappa.NN1]- (9CI) (CA INDEX NAME)

L20 ANSWER 3 OF 11 HCA COPYRIGHT 2003 ACS
135:344905 Catalysts containing n-pyrrolyl substituted nitrogen donors for olefin polymerization. Moody, Leslie Shane; MacKenzie, Peter Borden; Killian, Christopher Moore; Lavoie, Gino Georges; Ponasik, James Allen, Jr.; Smith, Thomas William; Pearson, Jason Clay; Barrett, Anthony Gerard Martin; Coates, Geoffrey William (Eastman Chemical Company, USA). PCT Int. Appl. WO 2001083571 A2 20011108, 355 pp. DESIGNATED STATES: W: CA, CN, JP, MX; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US13643 20010427. PRIORITY: US 2000-563812 20000503.
AB Catalyst compns. useful for the polymn. or oligomerization of olefins, comprises a Ti, Zr, or Hf complex of a dianionic bidentate ligand, wherein

at least one of the donor atoms of the ligand is a nitrogen atom substituted by a 1-pyrrolyl or 5 substituted 1-pyrrolyl group, wherein the remaining donor atoms of the ligand are selected from the group consisting of C, N, P, As, O, S, and Se.

289708-74-3P 289708-75-4P 289708-76-5P

289708-77-6P 289708-81-2P 289708-82-3P

289708-83-4P 289708-84-5P 289708-85-6P

289708-87-8P 289708-89-0P 289708-91-4P

289708-93-6P 289708-95-8P 289708-96-9P

371971-47-0P 371971-48-1P 371971-49-2P

371971-50-5P 371971-51-6P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(catalysts contg. n-pyrrolyl substituted nitrogen donors for olefin polymn.)

RN 289708-74-3 HCA

ΙT

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-75-4 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-76-5 HCA

CN 'Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-77-6 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-

bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-81-2 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-82-3 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-83-4 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)dimethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-84-5 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)dimethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-85-6 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-diphenyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-87-8 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-diphenyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-89-0 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-(1,1-dimethylethyl)-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-91-4 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)dimethylidyne]bis[2-(1,1-dimethylethyl)-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-93-6 HCA

RN 289708-95-8 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-(1-methylethyl)-5-(2-methylphenyl)-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-96-9 HCA

CN Iron, trichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 371971-47-0 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,6-dimethyl-1-piperidinamine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 371971-48-1 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[4-morpholinamine-.kappa.NN4]]- (9CI) (CA INDEX NAME)

RN 371971-49-2 HCA

CN Cobalt, dichloro[N, N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[4-

morpholinamine-.kappa.NN4]]- (9CI) (CA INDEX NAME)

RN 371971-50-5 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[4-methyl-l-piperazinamine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 371971-51-6 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[4-methyl-1-piperazinamine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

L20 ANSWER 4 OF 11 HCA COPYRIGHT 2003 ACS

135:304267 Production of supported catalysts for polymerization of olefins.
Kristen, Marc Oliver; Hauck, Gerhard; Gonioukh, Andrei; Sueling, Carsten;
Spaether, Wolf (Basf AG, Germany). Ger. Offen. DE 10017666 A1 20011011,
24 pp. (German). CODEN: GWXXBX. APPLICATION: DE 2000-10017666 20000408.

AB Supported catalysts for polymn. of olefins are manufd. by depositing transition metal complexes of 5- or 6-membered-ring-based heterocyclic compds. and activators based on Group IIIA element compds. on water-free, porous supports.

IT 328239-72-1

RL: CAT (Catalyst use); USES (Uses)
(prodn. of catalysts based on supported mixts. of transition metal
complexes of five- or six-membered ring-based heterocyclic compds. and
Group IIIA element compds. for polymn. of olefins)

RN 328239-72-1 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

L20 ANSWER 5 OF 11 HCA COPYRIGHT 2003 ACS

135:304266 Production of supported catalysts for polymerization of olefins. Kristen, Marc Oliver; Hauck, Gerhard (Basf AG, Germany). Ger. Offen. DE 10017663 A1 20011011, 22 pp. (German). CODEN: GWXXBX. APPLICATION: DE 2000-10017663 20000408.

AB Supported catalysts for polymn. of olefins are manufd. by depositing transition metal complexes of 5- or 6-membered-ring-based heterocyclic compds. and activators based on Group IIIA element compds. on porous supports contg. 2-10% water.

IT 328239-72-1

RL: CAT (Catalyst use); USES (Uses)
(prodn. of catalysts based on supported mixts. of transition metal
complexes of five- or six-membered ring-based heterocyclic compds. and
Group IIIA element compds. for polymn. of olefins)

RN 328239-72-1 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

L20 ANSWER 6 OF 11 HCA COPYRIGHT 2003 ACS

135:289197 Procedure for the production of a catalyst system for the polymerization of olefins. Kristen, Marc Oliver; Hauck, Gerhard (Basf AG, Germany). Ger. Offen. DE 10017660 Al 20011011, 14 pp. (German). CODEN: GWXXBX. APPLICATION: DE 2000-10017660 20000408.

AB Catalysts for polymn. of olefins are manufd. by mixing transition metal complexes of 5- or 6-membered heterocyclic compds. with activators based on Group IIIA compds. and then adding alkylating agents based on organolithium, organomagnesium or organoaluminum compds.

IT 328239-72-1

RL: CAT (Catalyst use); USES (Uses) (prodn. of catalyst systems contg. transition metal complexes with five- or six-membered ring-based heterocyclic compds., activators, and alkylating agents for polymn. of olefins)

RN 328239-72-1 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

L20 ANSWER 7 OF 11 HCA COPYRIGHT 2003 ACS

135:167062 Bis(imino)pyridyl iron and cobalt complexes: the effect of nitrogen substituents on ethylene oligomerization and polymerization. Britovsek, George J. P.; Gibson, Vernon C.; Kimberley, Brian S.; Mastroianni, Sergio; Redshaw, Carl; Solan, Gregory A.; White, Andrew J. P.; Williams, David J. (Department of Chemistry, Imperial College, London, SW7 2AY, UK). Journal of the Chemical Society, Dalton Transactions (10), 1639-1644 (English) 2001. CODEN: JCSDAA. ISSN: 1472-7773. Publisher: Royal Society of

Chemistry.

The synthesis and characterization of 2,6-bis(imino)pyridyl iron and cobalt complexes [(2,6-(RN:CMe)2C5H3N)MCl2] contg. nitrogen substituents of the type R = NPh2, NPhMe, NMe2 or 2,5-dimethylpyrrolyl are described. These complexes, in combination with the co-catalyst MAO, give active catalysts for the oligomerization or polymn. of ethylene. The catalytic activity is strongly affected by the substituents R and the polymn. conditions used. The polymer properties are also a function of the R substituents. With R = NPhMe or NMe2, toluene sol. .alpha.-olefins are obtained, whereas the bulkier substituents (R = NPh2 or 2,5-dimethylpyrrolyl) give low mol. wt. solid polyethylene.

IT 289708-74-3P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. and use of bis(imino)pyridyl iron and cobalt complexes for ethylene oligomerization and polymn.)

RN 289708-74-3 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

L20 ANSWER 8 OF 11 HCA COPYRIGHT 2003 ACS
134:208317 Bisimidino compounds, their transition metal complexes, and use of the latter as polymerization catalysts. Kristen, Marc Olivier; Gonioukh, Andrei; Lilge, Dieter; Lehmann, Stephan; Bildstein, Benno; Amort, Christoph; Malaun, Michael (BASF A.-G., Germany). PCT Int. Appl. WO 2001014391 A1 20010301, 53 pp. DESIGNATED STATES: W: JP, KR, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (German). CODEN: PIXXD2. APPLICATION: WO 2000-EP7657 20000808. PRIORITY: DE 1999-19939415 19990820.

GI

$$R^3$$
 R^4
 R^2
 R^2

The compds. have the general formula I [A = N, O, P, S; R1 = NR5R6; R2 =AΒ NR5R6, NR7R8, alkyl, aryl, cycloalkyl; R3, R4 = H, alkyl, aryl, cycloalkyl; NR5R6 forms an (un)substituted 5-, 6- or 7-membered ring, which can be annellated with (un) substituted 5- or 6-membered rings; R7, R8 = alkyl, aryl, cycloalkyl; n = 1, 2]. Thus, MeCOCH2CH2COCHMe2 was condensed with AcNHNH2 to give 53% 1-acetamido-2-isopropyl-5methylpyrrole, which was deacetylated and condensed 2:1 with 2,6-diacetylpyridine to give a diimine, which was complexed with FeCl2. Copolymn. of ethylene with 1-hexene in toluene in the presence of Me aluminoxane and the complex at 30.degree. for 1 h gave a copolymer with catalyst efficiency 980 g/mmol catalyst-h.

289708-74-3P 289708-75-4P 289708-76-5P IΤ 289708-77-6P 289708-81-2P 289708-82-3P 328239-71-0P 328239-72-1P 328239-73-2P 328239-74-3P 328239-75-4P 328239-76-5P 328239-77-6P 328239-78-7P 328239-79-8P 328239-81-2P

> RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of transition metal complexes with bisimidino ligands) 289708-74-3 HCA

RN CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-75-4 HCA CN

Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-76-5 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-77-6 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-81-2 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-82-3 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-71-0 HCA

CN Iron, trichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-72-1 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-73-2 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-74-3 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-(2-methylphenyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-75-4 HCA

CN. Cobalt, dichloro[N, N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-

methyl-5-(2-methylphenyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)(9CI) (CA INDEX NAME)

RN 328239-76-5 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-1H-indol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-77-6 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-1H-indol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-78-7 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[9H-carbazol-9-amine-.kappa.NN9]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-79-8 HCA

CN Cobalt, dichloro[N, N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[9H-carbazol-9-amine-.kappa.NN9]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 328239-81-2 HCA

CN Cobalt, dichloro[N,N'-[(2,5-thiophenediyl-.kappa.S)dimethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

IT 289708-96-9P 328239-80-1P

RN

CN

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of transition metal complexes with bisimidino ligands)
289708-96-9 HCA
Iron, trichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA

Pr-i
N
Cli-Pr
3+Fe
Cli-Pr
i-Pr
i-Pr

Me

INDEX NAME)

RN 328239-80-1 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[3,5-dimethyl-4H-1,2,4-triazol-4-amine-.kappa.NN4]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

L20 ANSWER 9 OF 11 HCA COPYRIGHT 2003 ACS

133:208316 Catalysts containing n-pyrrolyl substituted nitrogen donors for polymerization of olefins. Moody, Leslie Shane; Mackenzie, Peter Borden; Killian, Christopher Moore; Lavoie, Gino Georges; Ponasik, James Allen, Jr.; Barrett, Anthony Gerard Martin; Smith, Thomas William; Pearson, Jason Clay (Eastman Chemical Company, USA). PCT Int. Appl. WO 2000050470 A2 20000831, 368 pp. DESIGNATED STATES: W: CA, CN, JP, MX; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US4259 20000218. PRIORITY: US 1999-PV121135 19990222; US 1999-PV123276 19990308; US 1999-PV123385 19990308; US 1999-PV130503 19990423; US 1999-PV145277 19990726.

AB A catalyst compn. for the polymn. or oligomerization of olefins comprises a metal complex ligated by a monodentate, bidentate, tridentate, or tetradentate ligand, wherein at least one of the donor atoms of the ligand

is a 5 nitrogen atom substituted by a 1-pyrrolyl or substituted 1-pyrrolyl group; wherein: the remaining donor atoms of the ligand are selected from the group consisting of C, N, P, As, O, S, and Se; and wherein the metal in the metal complex is selected from the group consisting of Sc, Ta, Ti, Zr, Hf, V, Nb, Cr, Mo, W, Mn, Re, Fe, Ru, Os, Co, Rh, Ir, Ni, Cu, Pd, Pt, Al, 10 and Ga. Also disclosed are processes for the polymn. or oligomerization of olefins using the catalyst compns.

289708-74-3P 289708-75-4P 289708-76-5P 289708-77-6P 289708-81-2P 289708-82-3P 289708-83-4P 289708-84-5P 289708-85-6P 289708-87-8P 289708-89-0P 289708-91-4P 289708-93-6P 289708-95-8P 289708-96-9P 289708-98-1P

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(catalysts contg. n-pyrrolyl substituted nitrogen donors for polymn. of olefins)

RN 289708-74-3 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-75-4 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-76-5 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX

NAME)

RN 289708-77-6 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-81-2 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-82-3 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-methyl-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-83-4 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)dimethylidyne]bis[2,5-dimethyl-lH-pyrrol-l-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-84-5 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)dimethylidyne]bis[2,5-dimethyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-85-6 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-diphenyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-87-8 HCA

CN Cobalt, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-diphenyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-89-0 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-(1,1-dimethylethyl)-5-phenyl-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI) (CA INDEX NAME)

RN 289708-91-4 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)dimethylidyne]bis[2-(1,1-dimethylethyl)-5-(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]- (9CI)

(CA INDEX NAME)

RN 289708-93-6 HCA

CN Iron, dichloro[diethyl 1,1'-[(2,6-pyridinediyl-.kappa.N)]bis(methylidynenitrilo-.kappa.N)]bis[5-(1,1-dimethylethyl)-2-methyl-1H-pyrrole-3-carboxylate]]- (9CI) (CA INDEX NAME)

RN 289708-95-8 HCA

CN Iron, dichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2-(1-methylethyl)-5-(2-methylphenyl)-lH-pyrrol-l-amine-.kappa.NNl]]- (9CI) (CA INDEX NAME)

RN 289708-96-9 HCA

CN Iron, trichloro[N,N'-[(2,6-pyridinediyl-.kappa.N)diethylidyne]bis[2,5-bis(1-methylethyl)-1H-pyrrol-1-amine-.kappa.NN1]]-, (SP-5-31)- (9CI) (CA INDEX NAME)

RN 289708-98-1 HCA

CM 1

CRN 289708-97-0 CMF C29 H41 Fe N5

CCI CCS

CM 2

CRN 14874-70-5 CMF B F4 CCI CCS

L20 ANSWER 10 OF 11 HCA COPYRIGHT 2003 ACS

119:173002 2,6-Diacetylpyridinesalicylaldazine complexes of bivalent metal ions. Singh, Bachcha; Singh, Udai R. (Dep. Chem., Banaras Hindu Univ., Varanasi, 221 005, India). Transition Metal Chemistry (Dordrecht, Netherlands), 18(4), 413-16 (English) 1993. CODEN: TMCHDN. ISSN: 0340-4285.

AB 2,6-Diacetylpyridinesalicylaldazine (H2daps) formed [Ni(H2daps)C1H2O]C1, [M(H2daps)C12H2O] (M = Mn, Co, Cu, Zn) and [M'(daps)(H2O)2] (M' = Mn, Co, Ni, Cu, Zn) which were characterized by elemental anal., physicochem. methods, spectroscopy, and x-ray powder diffraction.

IT 150265-13-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn and x-ray diffraction and thermal decompn. of)

RN 150265-13-7 HCA

CN Nickel(1+), aquachloro[2-hydroxybenzaldehyde (2,6-pyridinediyldiethylidyne)dihydrazone]-, chloride (9CI) (CA INDEX NAME)

• c1-

RN 150265-20-6 HCA

CN Manganese, aquadichloro[2-hydroxybenzaldehyde (2,6-pyridinediyldiethylidyne)dihydrazone]- (9CI) (CA INDEX NAME)

RN 150265-21-7 HCA

CN Cobalt, aquadichloro[2-hydroxybenzaldehyde (2,6-pyridinediyldiethylidyne)dihydrazone]- (9CI) (CA INDEX NAME)

RN 150265-22-8 HCA

CN Copper, aquadichloro[2-hydroxybenzaldehyde (2,6-pyridinediyldiethylidyne)dihydrazone]- (9CI) (CA INDEX NAME)

L20 ANSWER 11 OF 11 HCA COPYRIGHT 2003 ACS

107:69597 Synthesis and characterization of lanthanon complexes with bis(o-hydroxyacetophenone)-2,6-dipicolinoyldihydrazone. Arora, D. L.; Lal, Keemti; Gupta, S. P. (Dep. Chem., D. N. Coll., Meerut, 250 002, India). Journal of the Indian Chemical Society, 63(9), 836-8 (English) 1986. CODEN: JICSAH. ISSN: 0019-4522.

AB [Ln2LC13(H2O)2]Cl (I; Ln = La, Ce, Pr, Nd, Sm; H2L = bis(o-hydroxyacetophenone)-2,6-dipicolinoyldihydrazone) were prepd. from LnCl3 and H2L in aq. EtOH. I were characterized by IR and electronic spectra, magnetic moment and elec. cond. measurements. Ligand field parameters were calcd. for the Pr, Nd, and Sm complexes. The hydrazone is heptadentate, coordinating through the pyridine N, 2 azomethine N, 2 secondary amide N, and 2 phenolic O atoms. The environments of both Ln atoms are 6-coordinate and 1 Ln atom is present as LnN3L3 and the other as LnN2O4.

IT 109612-46-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and ligand field parameters of)

RN 109612-46-6 HCA

CN Lanthanum(1+), diaquatrichloro[.mu.-[[2,6-pyridinedicarboxylic acid bis[[1-(2-hydroxyphenyl)ethylidene]hydrazidato]](2-)]]di-, chloride (9CI) (CA INDEX NAME)

=> d L32 1-6 cbib abs hitstr

L32 ANSWER 1 OF 6 HCA COPYRIGHT 2003 ACS
133:173325 Potentialities of some newly synthesized organophosphorus
derivatives as fungicides against sugarcane pathogens. Sengupta, S. K.;
Pandey, O. P.; Rao, G. P. (Chemistry Department, D.D.U. Gorakhpur

University, Gorakhpur, 273 009, India). Sugarcane Pathology, Volume 1, 279-300. Editor(s): Rao, Govind P. Science Publishers, Inc.: Enfield, N.

H. (English) 1999. CODEN: 69ABB7.

- The antifungal assay of organophosphorus derivs. contg. bis(mercapto AB triazoles), bis(mercapto thiadiazoles), bis(mercapto oxadiazoles), alkyl xanthates, thiosemicarbazones, dithiocarbazates, mercaptotriazines, mercaptotriazoles and thiohydantoins was carried out. Ninety-eight newly synthesized organophosphorus derivs., belonging to the above-mentioned series were screened for their antifungal efficacy against many fungal pathogens of sugarcane. O, O-Di-Et thiophosphate derivs. contg. bis(mercaptotriazoles) exhibited abs. inhibition against Colletotrichum falcatum, Fusarium oxysporum and Curvularia pallescens, at 1000 ppm. 1,2-Bis(5-mercapto-1,3,4-triazol-2-yl)ethane was 100% antifungal against C. falcatum, even at 100 ppm. Organophosphorus derivs. contg. bis(mercapto triazoles) were more effective, as compared to derivs. contg. bis(mercaptothiadiazoles) or bis(mercaptooxadiazoles). The O,O-di-Et thiophosphate derivs. contg. alkyl xanthates exhibited 100% mycelial inhibition against all the test fungi, at 1000 ppm. Among organophosphorus derivs. contg. substituted thiosemicarbazones, the O,O-di-Et phosphate derivs. of 2-acetylpyridine-4-(4chlorophenyl)thiosemicarbazone and 2,6-diacetylpyridinebis(chlorophenylthi osemicarbazone) showed complete mycelial inhibition of all the test fungi at 1000 ppm. The organophosphorus derivs. of dithiocarbazates were found to be poor, as compared to derivs. of thiosemicarbazones. The best results were achieved with organophosphorus derivs. of mercaptotriazoles. The derivs. of substituted mercaptotriazines were less effective than mercaptotriazole derivs. The organophosphorus derivs. of substituted thiohydantoins also showed promising results in inhibiting the mycelial growth of all the test fungi. All these compds. were also found superior to many com. fungicides viz., Bavistin, Blitox-50, Topsin-M, Dithane M-45.
- IT 288612-89-5 288612-90-8 288612-91-9

288612-92-0 288612-94-2

- RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses) (fungicidal activity against sugarcane pathogens)
- RN 288612-89-5 HCA
- CN Phosphorothious acid, S,S'-[2,6-pyridinediylbis[ethylidynenitrilo(5-phenyl-4H-1,2,4-triazole-4,3-diyl)]] O,O,O',O'-tetraethyl ester (9CI) (CA INDEX NAME)

RN 288612-90-8 HCA

CN Phosphorothious acid, S,S'-[2,6-pyridinediylbis[ethylidynenitrilo[5-(2-chlorophenyl)-4H-1,2,4-triazol-5,3-diyl]]] O,O,O',O'-tetraethyl ester (9CI) (CA INDEX NAME)

RN 288612-91-9 HCA

CN Phosphorothious acid, S,S'-[2,6-pyridinediylbis[ethylidynenitrilo[5-(4-chlorophenyl)-4H-1,2,4-triazol-5,3-diyl]]] O,O,O',O'-tetraethyl ester (9CI) (CA INDEX NAME)

RN 288612-92-0 HCA

CN Phosphorothious acid, S,S'-[2,6-pyridinediylbis[ethylidynenitrilo[5-(4-nitrophenyl)-4H-1,2,4-triazol-5,3-diyl]]] O,O,O',O'-tetraethyl ester (9CI) (CA INDEX NAME)

RN 288612-94-2 HCA

CN Phosphorothioic acid, S,S'-[2,6-pyridinediylbis[ethylidynenitrilo(6-methyl-5-oxo-1,2,4-triazin-4,3(5H)-diyl)]] O,O,O',O'-tetraethyl ester (9CI) (CA INDEX NAME)

L32 ANSWER 2 OF 6 HCA COPYRIGHT 2003 ACS

108:123994 Identification of a reactive intermediate of furazolidone formed by swine liver microsomes. Vroomen, Louis H. M.; Groten, John P.; Van Muiswinkel, Kees; Van Velduizen, Albertus; Van Bladeren, Peter J. (Dep. Toxicol., State Inst. Qual. Control Agric. Prod., Wageningen, 6708 PD, Neth.). Chemico-Biological Interactions, 64(1-2), 167-79 (English) 1987. CODEN: CBINA8. ISSN: 0009-2797.

Furazolidone [N-(5-nitro-2-furfurylidene)-3-amino-2-oxazolidone] is AΒ metabolized by swine liver microsomes under aerobic and anaerobic conditions. Covalent binding to microsomal protein amounted aerobically to 0.29 nmol/mg protein/min. Of all amino acids tested, only addn. of cysteine to the incubation mixt. decreased microsomal protein binding of furazolidone, indicating that covalent binding may occur at protein thiol groups. Two known metabolites of furazolidone, 3-(4-cyano-2-oxobutylideneamino)-2-oxazolidone and 2,3 dihydro-3-cyanomethyl-2-hydroxyl-5-nitro-1.alpha., 2-di(2-oxo-oxazolidin-3-yl) iminomethyl-furo[2,3-b] furan, were minor metabolites. At least 50% of total metabolites is formed by swine liver microsomes via a reductive process of furazolidone as indicated by the formation of a furazolidone-mercaptoethanol conjugate after the addn. of mercaptoethanol to the incubation mixt. The conjugate was identified as 3-(4-cyano-3-.beta.-hydroxyethylmercapto-2-oxobutylidene amino)-2-oxazolidone, indicating that the open-chain acrylonitrile-deriv. is the reactive intermediate of furazolidone which also may be responsible for interaction with protein.

IT 77940-44-4

RL: BIOL (Biological study)

(furazolidone metabolite, formation of, in liver microsomes of swine)

RN 77940-44-4 HCA

CN Furo[2,3-b]furan-3-acetonitrile, 2,3,3a,6a-tetrahydro-2-hydroxy-5-nitro-2,6a-bis[[(2-oxo-3-oxazolidinyl)imino]methyl]- (9CI) (CA INDEX NAME)

L32 ANSWER 3 OF 6 HCA COPYRIGHT 2003 ACS

107:89217 Quantitative studies of the metabolism of furazolidone by rat liver
 microsomes. Vroomen, L. H. M.; Van Ommen, B.; Van Bladeren, P. J.
 (Toxicol. Sect., State Inst. Quality Cont. Agric. Prod., Wageningen, 6708
 PD, Neth.). Toxicology in Vitro, 1(2), 97-104 (English) 1987. CODEN:
 TIVIEQ. ISSN: 0887-2333.

The in vitro aerobic and anaerobic metab. of furazolidone (I) by rat liver microsomes may be mediated by NADPH-cytochrome P 450 reductase. Two major metabolites, 3-(4-cyano-2-oxobutylideneamino)-2-oxazolidone (II) and 2,3-dihydro-3-cyanomethyl-2-hydroxy-5-nitro-1.alpha.,2-di(2-oxooxazolidin-3-yl)iminomethylfuro[2,3-b]furan (III), accounted for 16.6 and 16.4%, resp., of the total extractable radioactivity after incubation with [14C]I. II and III may derive from a common intermediate, possibly a nitroso or a hydroxylamine deriv. of I. During metab., 2-3% of the total metabolites became covalently bound to microsomal protein. The presence of reduced glutathione in the incubation mixt. inhibited this binding and prevented the metab. of I to II or III. Other minor metabolites of I were not characterized. No interaction of I with added calf thymus DNA was detected.

IT 77940-44-4

RL: FORM (Formation, nonpreparative)

(formation of, as furazolidone metabolite, by liver microsome)

RN 77940-44-4 HCA

CN Furo[2,3-b]furan-3-acetonitrile, 2,3,3a,6a-tetrahydro-2-hydroxy-5-nitro-2,6a-bis[[(2-oxo-3-oxazolidinyl)imino]methyl]- (9CI) (CA INDEX NAME)

L32 ANSWER 4 OF 6 HCA COPYRIGHT 2003 ACS

95:35191 Metabolism of furazolidone by milk xanthine oxidase and rat liver 9000g supernatant: formation of a unique nitrofuran metabolite and an aminofuran derivative. Tatsumi, Kiyoshi; Yamada, Hideyuki; Yoshimura, Hidetoshi; Kawazoe, Yuichi (Fac. Pharm. Sci., Kyushu Univ., Fukuoka, 812, Japan). Archives of Biochemistry and Biophysics, 208(1), 167-74 (English) 1981. CODEN: ABBIA4. ISSN: 0003-9861.

$$O_2N \longrightarrow CH = NN \longrightarrow O$$

$$O_2N \longrightarrow CH = NN \longrightarrow O$$

$$O_3N \longrightarrow CH = NN \longrightarrow O$$

$$O_3N \longrightarrow O$$

$$O_4N \longrightarrow O$$

$$O$$

AB In vitro metab. of furazolidone (I) [67-45-8] was investigated by using milk xanthine oxidase [9002-17-9] and rat liver 9000 g supernatant. As a result, a new type of redn. product was isolated as one of the main metabolites from the incubation mixt. and it was tentatively identified as 2,3-dihydro-3-cyanomethyl-2-hydroxyl-5-nitro-1a,2-bis(2-oxooxazolidin-3-yl)iminomethylfuro[2,3-b]furan (II) [77940-44-4]. In addn., the formation of N-(5-amino-2-furfurylidene)-3-amino-2-oxazolidone [13641-84-4], a minor metabolite of nitrofuran, in a milk xanthine oxidase system was also demonstrated. The aminofuran deriv. was easily degraded by milk xanthine oxidase under aerobic, but not anaerobic, conditions. The degrdn. appears to be due to superoxide anion radicals, hydroxyl radicals, and(or) singlet O, which are produced in this enzyme system.

IT 77940-44-4

RL: BIOL (Biological study)
 (as furazolidone metabolite)

RN 77940-44-4 HCA

CN Furo[2,3-b] furan-3-acetonitrile, 2,3,3a,6a-tetrahydro-2-hydroxy-5-nitro-2,6a-bis[(2-oxo-3-oxazolidinyl)imino]methyl]- (9CI) (CA INDEX NAME)

L32 ANSWER 5 OF 6 HCA COPYRIGHT 2003 ACS

72:55178 Syntheses in the pyridine series. IV. Condensation of diformylpyridines and 2,4,6-triformylpyridine with aromatic amines, hydrazines, and other hydrogen-containing active compounds. Queguiner, Guy; Pastour, Paul (Inst. Nat. Super. Chim. Ind. Rouen, Mont-Saint-Aignan, Fr.). Bulletin de la Societe Chimique de France (10), 3659-62 (French) 1969. CODEN: BSCFAS: ISSN: 0037-8968.

GI For diagram(s), see printed CA Issue.

AB Formylpyridines (I) are treated with anilines, naphthylamines, N-aminopyrrolidine, -piperidine, and -morpholine, and HONH2 to give bis-(iminomethyl)pyridines (II). Similarly prepd. are III.

IT 25242-34-6P 25242-42-6P
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of) RN 25242-34-6 HCA

CN Pyridine, 2,6-bis(N-1-pyrrolidinylformimidoyl) - (8CI) (CA INDEX NAME)

$$N-N$$
 $CH-N$ $CH-N$

RN 25242-42-6 HCA

CN Pyridine, 2,4,6-tris(N-1-pyrrolidinylformimidoyl) - (8CI) (CA INDEX NAME)

L32 ANSWER 6 OF 6 HCA COPYRIGHT 2003 ACS

55:65067 Original Reference No. 55:12409g-i,12410a-b Alkylidene- and arylideneaminomorpholines. Wiley, Richard H.; White, H. Keith; Irick, Gether (Univ. of Louisville, Louisville, KY). J. Org. Chem., 24, 1784-6 (Unavailable) 1959. CODEN: JOCEAH. ISSN: 0022-3263.

GI For diagram(s), see printed CA Issue.

cf. CA 51, 14717a. Concd. aq. NH3 (13.4 ml.) added slowly with gentle swirling to 161 g. 5.25% com. aq. NaOCl at 0-2.degree., after 5 min. in the ice bath the soln. treated at once with 11.5 g. morpholine, allowed to warm slowly to room temp. during 6 hrs. with occasional swirling, and the ppt. (0.25 g. 4,4'-azomorpholine, m. 151.degree.) filtered off gave an aq. filtrate (I) contg. 4-aminomorpholine. I concd. in vacuo on a steam bath to 100 ml., dild. with 100 ml. MeOH, after 15 min. filtered, the filtrate treated with 7.68 g. 2-MeOC6H4CHO, the mixt. refluxed 2 hrs., kept overnight, and the product collected gave 11.9 g.

O.CH2.CH2.N(N:CHR).CH2.CH2 (II) (R = C6H4OMe-2) (III), m. 76-7.degree. (EtOH). I (twice the amt. prepd. above) acidified with concd. HCl to the point where the soln. turned from colorless to bright yellow, treated with

point where the soln. turned from colorless to bright yellow, treated with 10 g. Et2CHCHO, refluxed 2 hrs., extd. with Et2O, the aq. soln. made strongly alk. with concd. aq. NH3, and the product isolated with Et2O gave

7.65 g. II (R = CHEt2), b1 69.degree., n25D 1.4746. The following II were prepd. similarly (R, % yield, and m.p. given): iso-Bu, 37, -(b9 100.degree., n25D 1.4739); (CH2)5Me, -, -(b6 126.degree., n26D 1.4746); Ph, -, 89.degree. (aq. EtOH); C6H4NHAC-4, 77, 206.degree. (aq. MeOH); C6H4Cl-4, -, 99.degree. (EtOH); C6H3(OEt)2-3,4, 90, 99.degree. (aq. MeOH); C6H4NMe2-4, 58, 166.degree. (aq. EtOH); C6H4NO2-3, 90, 153.degree. (aq. EtOH); 1-naphthyl, 67, 63.degree. (aq. EtOH); 2-hydroxy-1-naphthyl, 73, 121.degree. (aq. MeOH); 9-anthryl, 58, 193.degree. (aq. EtOH); 2-pyridyl, 44, 47-56.degree. (b0.15 118.degree.); 6-methyl-2-pyridyl, 35, 53-7.degree. (b1 168.degree.); 6-formyl-2-pyridyl, 32, 136.degree. (aq. MeOH). III showed no strong or consistent activity in tests on exptl. mouse sarcoma 180. Other compds. showed no evidence of tumor growth retardation. The infrared absorption characteristics of the compds. were reported.

IT 109443-72-3, Morpholine, 4,4'-[2,6-pyridinediylbis(methylidynenitrilo)]di-

(prepn. of)

RN 109443-72-3 HCA

CN Morpholine, 4,4'-[2,6-pyridinediylbis(methylidynenitrilo)]di- (6CI) (CA INDEX NAME)

$$\bigcirc N - N = CH - N - N \bigcirc CH = N$$

=> d L36 1 cbib abs fhitstr

Balance of answers.

L36 ANSWER 1 OF 25 HCA COPYRIGHT 2003 ACS

138:122642 Preparation of 5-substituted indeno[1,2-c]pyrazol-4-ones as anti-cancer and anti-proliferative agents. Nugiel, David; Carini, David; Dimeo, Susan; Vidwans, Anup; Yue, Eddy (Bristol-Myers Squibb Pharma Company, USA). PCT Int. Appl. WO 2003007883 A2 20030130, 184 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-US22663 20020716. PRIORITY: US 2001-906963 20010716.

GI

AB The title compds. [I; X = O, S, NR (wherein R = H, alkyl, (un)substituted NH2); R1 = H, (un)substituted alkyl, alkenyl, etc.; R2 = H, (un)substituted alkyl, alkenyl, etc.] that are potent inhibitors of the class of enzymes known as cyclin dependent kinases, which relate to the catalytic subunits cdkl-7 and their regulatory subunits known as cyclines A-G and therefore are useful in treating cancer or other proliferative diseases (no data), were prepd. E.g., a 3-step synthesis of indeno[1,2-c]pyrazol-4-one II, starting with di-Me 3-nitrophthalate, was given.

IT 247149-71-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 5-substituted indeno[1,2-c]pyrazol-4-ones as anti-cancer and anti-proliferative agents)

RN 247149-71-9 HCA

CN

2-Thiophenecarboxamide, 5-[2,4-dihydro-5-[[(4-morpholinylamino)carbonyl]amino]-4-oxoindeno[1,2-c]pyrazol-3-yl]-N-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

=> d L36 2 cbib abs fhitstr

L36 ANSWER 2 OF 25 HCA COPYRIGHT 2003 ACS
135:288778 Preparation of indeno[1,2-c]pyrazol-4-ones as inhibitors of cyclin dependent kinases. Nugiel, David A.; Carini, David J.; Dimeo, Susan V.; Yue, Eddy W. (USA). U.S. Pat. Appl. Publ. US 20010027195 A1 20011004, 104

Rip Lee

pp., Cont.-in-part of U.S. Ser. No. 639,618. (English). CODEN: USXXCO.
APPLICATION: US 2000-731304 20001206. PRIORITY: US 1998-PV82476 19980421;
US 1999-295078 19990420; US 2000-639618 20000815.

GI

AΒ The present invention relates to the synthesis of a new class of indeno[1,2-c]pyrazol-4-ones of formula [X = 0, S, (un)substituted NH; R1 = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, NH2, C3-10 membered carbocyclyl, 3-10 membered heterocycle contg. 1-4 heteroatoms selected from O, N, and S; R2 = H, (un)substituted C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, (CF2)mCF3, C3-10 membered carbocyclyl, 3-10 membered heterocycle contg. 1-4 heteroatoms selected from O, N, and S; wherein m = 0, 1-4]. These compds. are potent inhibitors of the class of enzymes known as cyclin dependent kinases, which relate to the catalytic subunits cdk1-9 and their regulatory subunits know as cyclins A-H. invention also provides a novel method of treating cancer or other proliferative diseases by administering a therapeutically effective amt. of one of these compds. or a pharmaceutically acceptable salt form thereof. Alternatively, cancer or other proliferative diseases can be treated by administering a therapeutically effective combination of one of the compds. of the present invention and one or more other known anti-cancer or anti-proliferative agents (no data). Thus, hydrogenation of di-Me 3-nitrophthalate over 5% Pd-C in methanol in a Parr shaker at 50 psi for 2 h followed by acetylation with Ac2O in pyridine at 25.degree. for 2 h gave 79% di-Me 3-acetamidophthalate which was treated with NaH in DMF and cyclocondensed with 4-methoxyacetophenone at 90.degree. for 20 min to give 30% 2-(4-methoxybenzoyl)-4-acetamidoindane-2,3-dione. Cyclocondensation of the latter triketone with hydrazine hydrate in the presence of p-TsOH in ethanol under reflux for 2 h gave I (R1 = Me, X = O, R2 = 4-methoxyphenyl).

IT 247149-77-5P

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of indeno[c]pyrazolones as inhibitors of cyclin dependent kinases)

RN 247149-77-5 HCA

2-Thiophenecarboxamide, 5-[2,4-dihydro-5-[[(4-morpholinylamino)carbonyl]amino]-4-oxoindeno[1,2-c]pyrazol-3-yl]-N-4-morpholinyl- (9CI) (CA INDEX NAME)

=> d L36 3-25 cbib abs fhitstr

L36 ANSWER 3 OF 25 HCA COPYRIGHT 2003 ACS

131:299444 Preparation of 5-aminoindeno[1,2-c]pyrazol-4-ones as anti-cancer and anti-proliferative agents. Nugiel, David A.; Carini, David J.; Yue, Eddy W.; Dimeo, Susan V. (Du Pont Pharmaceuticals Company, USA). PCT Int. Appl. WO 9954308 A1 19991028, 184 pp. DESIGNATED STATES: W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US8616 19990420. PRIORITY: US 1998-82476 19980421.

GΙ

The title compds. [I; X = O, S, NR (wherein R = H, alkyl, (un)substituted NH2); Rl = H, (un)substituted alkyl, alkenyl, etc.; R2 = H, (un)substituted alkyl, alkenyl, etc.] that are potent inhibitors of the class of enzymes known as cyclin dependent kinases, which relate to the catalytic subunits cdkl-7 and their regulatory subunits known as cyclines A-G and therefore are useful in treating cancer or other proliferative diseases (no data), were prepd. E.g., a 3-step synthesis of indeno[1,2-c]pyrazol-4-one II, starting with di-Me 3-nitrophthalate, was given. Alternatively, one can treat cancer or other proliferative diseases by administering a therapeutically effective combination of one of the compds.I and one or more other known anti-cancer or

anti-proliferative agents.

IT 247149-71-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 5-aminoindeno[1,2-c]pyrazol-4-ones as anti-cancer and anti-proliferative agents)

RN 247149-71-9 HCA

CN 2-Thiophenecarboxamide, 5-[2,4-dihydro-5-[[(4-morpholinylamino)carbonyl]amino]-4-oxoindeno[1,2-c]pyrazol-3-yl]-N-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

L36 ANSWER 4 OF 25 HCA COPYRIGHT 2003 ACS

130:338001 Synthesis of new potential bis-intercalators based on chiral pyridine-2,6-dicarboxamides. Amr, Abd El-Galil; Abd El-Salam, Osama I.; Attia, Abd El-Hamid; Stibor, Ivan (Department of Organic Chemistry, National Research Centre, Cairo, 12622, Egypt). Collection of Czechoslovak Chemical Communications, 64(2), 288-298 (English) 1999. CODEN: CCCCAK. ISSN: 0010-0765. OTHER SOURCES: CASREACT 130:338001. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

AB Potential bis-intercalating compds. N, N-dibenzylidene-N2, N2'-(pyridine-2, 6-dicarbonyl) di(amino acid hydrazides), N, N'-substituted pyridine-2, 6-bis(hydrazides) and N, N'-substituted N2N2'-bis(pyridine-2, 6-dicarbonyl)di(amino acid hydrazides), both racemic and optically active, can be easily synthesized from pyridine-2, 6-bis(hydrazide), natural amino acids and arom. aldehydes or anhydrides of arom. ortho-dicarboxylic acids.

IT 224452-51-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and DNA intercalating properties of pyridinedicarboxamide
 derivs.)

RN 224452-51-1 HCA

CN 2,6-Pyridinedicarboxamide, N,N'-bis(2,5-dioxo-1-pyrrolidinyl)- (9CI) (CA INDEX NAME)

L36 ANSWER 5 OF 25 HCA COPYRIGHT 2003 ACS

130:311815 Preparation of pyrazole derivatives as calcium release-dependent calcium channel inhibitors and inhibitors of interleukin-2 (IL-2) production. Kubota, Hirokazu; Yonetoku, Yasuhiro; Sugasawa, Keizou; Funatsu, Masashi; Kawazoe, Souichirou; Toyoshima, Akira; Okamoto, Yoshinori; Ishikawa, Jun; Takeuchi, Makoto (Yamanouchi Pharmaceutical Co., Ltd., Japan). PCT Int. Appl. WO 9919303 A1 19990422, 54 pp. DESIGNATED STATES: W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1998-JP4583 19981012. PRIORITY: JP 1997-279093 19971013.

GΙ

AB Pyrazole derivs. represented by general formula [I; ring D = pyrazolyl optionally substituted by 1-3 substituents selected from alkyl, lower alkenyl, lower alkynyl, lower haloalkyl, cycloalkylalkyl, alkoxyalkyl, cycloalkyl, alkoxy, CO2H, alkoxycarbonyl, and halo; ring B = phenylene, a nitrogen-contg., divalent, satd. ring group, or an optionally alkylated, monocyclic, divalent heteroarom. ring group; X = -NR1-CR2R3-, -CR2R3-NR1-, -NR1-SO2-, -SO2-NR1- or -CR4:CR5-; wherein R1 = H, OH, alkyl, alkoxy, alkylcarbonyl; R2, R3 = H or alkyl or R2R3 = O or S; R4, R5 = H, halo, lower haloalkyl; A = (1) Ph optionally having one or more substituents,

(2) mono-, di- or tricyclic fused heteroaryl optionally having one or more substituents, (3) cycloalkyl optionally having one or more substituents, (4) a nitrogen-contg., satd. ring group optionally having one or more substituents, (5) lower alkenyl optionally having one or more substituents, (6) lower alkynyl optionally having one or more substituents, or (7) alkyl optionally having one or more substituents; or A and X are combined together to represent 1-pyrrolidinylcarbonyl, pyrazolidinylcarbonyl, piperidinocarbonyl, piperazinylcarbonyl, morpholinocarbonyl, 3,4-2H-1,4-benzoxazin-4-ylcarbonyl, or indolylcarbonyl] are prepd. Also claimed are medicinal compns., in particular, calcium release-dependent calcium channel inhibitors, IL-2 prodn. inhibitors, and therapeutics or preventives for allergies, inflammations, or autoimmune diseases, bronchial asthma, or rheumatoid arthritis for contg. the above compds. I as the active ingredients. Thus, 4-methylthiazole-5-carboxylic acid was condensed with 4-[3,5bis(trifluoromethyl)-1H-pyrazol-1-yl]aniline using 1-ethyl-3-(3dimethylaminopropyl)carbodiimide hydrochloride in 1,2-dichloroethane at room temp. overnight to give the title compd., 4'-pyrazolylthiazole-5carboxanilide deriv. (II). II in vitro showed IC50 of .ltoreq.1 .mu.M .mu.g/mL for inhibiting the prodn. of IL-2 in Jurkat cells.

IT 223499-79-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrazole derivs. as calcium release-dependent calcium channel inhibitors and inhibitors of interleukin-2 prodn. for treatment and prevention of diseases)

223499-79-4 HCA

2-Thiophenecarboxamide, 5-[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]-N-4H-1,2,4-triazol-4-yl- (9CI) (CA INDEX NAME)

L36 ANSWER 6 OF 25 HCA COPYRIGHT 2003 ACS

130:281952 Pyrroloindoles. 17. Synthesis and condensation reactions of
 benzo[e]pyrrolo[3,2-g]indole-2,9-dicarboxylic acid dichloride. Samsoniya,
 Sh. A.; Trapaidze, M. V.; Kuprashvili, N. A.; Zurabishvili, D. S.;
 Suvorov, N. N. (Iv. Dzhavakhishvili State University, Tbilisi, 380028,
 Georgia). Chemistry of Heterocyclic Compounds (New York) (Translation of
 Khimiya Geterotsiklicheskikh Soedinenii), Volume Date 1998, 34(7), 816-821
 (English) 1999. CODEN: CHCCAL. ISSN: 0009-3122. OTHER SOURCES: CASREACT
 130:281952. Publisher: Consultants Bureau.

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RN

CN

AB Benzopyrroloindoledicarboxylic acid dichloride I (R = Cl) was prepd. and condensed with amines and phenols to give the corresponding diamides and activated diesters I [R = PhNH, 4-ClC6H4NH, adamantylamino, 1-piperazinyl, 4-MeN(CH2CH2)2N, 2-HO2CC6H4NH, 4-H2NSO2C6H4NH, Me2N, 4-pyridinylcarbonylhydrazinyl, Cl5C6O, 4-O2NC6H4O, 2,4-(O2N)2C6H3]. The mass spectra of the dichloride and several diamides have been investigated.

IT 222983-81-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of diamides and diesters of benzopyrroloindoledicarboxylic acid by condensation reactions of the acid dichloride with amines and phenols)

RN 222983-81-5 HCA

CN Benzo[e]pyrrolo[3,2-g]indole-2,9-dicarboxamide, 1,10-dihydro-N,N'-bis(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

L36 ANSWER 7.0F 25 HCA COPYRIGHT 2003 ACS

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130:223303 Preparation of 5H-pyrrolo[2,1-c][1,4]benzodiazepine-3-carboxamides as vasopressin V2 receptor antagonists. Trybulski, Eugene J.; Molinari, Albert J.; Bagli, Jehan F.; Ashwell, Mark A.; Caggiano, Thomas J. (American Home Products Corporation, USA). U.S. US 5880122 A 19990309, 122 pp. (English). CODEN: USXXAM. APPLICATION: US 1997-955511 19971022.

·GI

Ι

AB Title compds. [I; R = OH, NR1R3, ZR1, etc.; R1 = H or alkyl; R3 = aminoalkyl, pyridylalkyl, imidazolylalkyl; R4, R5 = H, halo, alkyl, alkoxy, etc.; R6 = COZ1NR1COR7; R7 = cycloalkyl, 2-(hetero)arylphenyl(methyl), 2-(hetero)aryl-3-pyridyl(methyl), etc.; Z = piperazine-1, 4-diyl; Z1 = (un)substituted 1,4-phenylene or -pyridine-3,6-diyl] were prepd. Thus, Me 4-amino-2-methoxybenzoate was amidated by 2-PhC6H4CO2H and the product amidated by 10,11-dihydro-5H-pyrrolo[2,1-c][1,4]benzodiazepine to give, in 3 addnl. steps, I (R = 4-methyl-1-piperazinyl, R4 = R5 = H, R6 = COZ1NHCOCH2Ph-2, Z1 = 2-methoxy-1,4-phenylene). Data for biol. activity of I were given.

IT 207670-29-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 5H-pyrrolo[2,1-c][1,4]benzodiazepine-3-carboxamides as vasopressin V2 receptor antagonists)

RN 207670-29-9 HCA

CN

5H-Pyrrolo[2,1-c][1,4]benzodiazepine-3-carboxamide, 10-[4-[([1,1'-biphenyl]-2-ylcarbonyl)amino]-2-chlorobenzoyl]-10,11-dihydro-N-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

L36 ANSWER 8 OF 25 HCA COPYRIGHT 2003 ACS

129:16147 Preparation of 5H-pyrrolo[2,1-c][1,4]-benzodiazepine-3-carboxamides as vasopressin V2 antagonists. Trybulski, Eugene John; Molinari, Albert John; Bagli, Jehan Framroz; Ashwell, Mark Anthony; Caggiano, Thomas Joseph

(American Home Products Corp., USA). PCT Int. Appl. WO 9820011 A1 19980514, 74 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US18918 19971022. PRIORITY: US 1996-743443 19961101.

GI

Title compds. [I; R3 = COR; R = (4-alkyl)-1-piperazinyl, 4-(di)(alkyl)amino-1-piperidinyl, (di)(alkyl)hydrazino, etc.; R4,R5 = H, halo, alkyl, alkoxy, etc.; R6 = COZR9; R9 = aroylamino, [(arylmethyl)carbonyl]amino, etc.; Z = (un)substituted 1,4-phenylene or -pyridinediyl] were prepd. Thus, 2-PhC6H4CO2H was amidated by 2,4-(MeO)(H2N)C6H3CO2Me and the sapond. product used to N-acylate 10,11-dihydro-5H-pyrrolo[2,1-c][1,4]benzodiazepine to give I (R4 = R5 = H, R6 = COZNHCOC6H4Ph-2, Z = 3-methoxy-1,4-phenylene)(II; R3 = H) which was acylated by Cl3CCOCl and the product hydrolyzed to give II (R3 = COR)(III; R = OH). The latter was amidated by 1-methylpiperazine to give III (R = 4-methyl-1-piperazinyl). Data for biol. activity of I were given.

IT 207670-29-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 5H-pyrrolo[2,1-c][1,4]-benzodiazepine-3-carboxamides as vasopressin V2 antagonists)

RN 207670-29-9 HCA

CN

5H-Pyrrolo[2,1-c][1,4]benzodiazepine-3-carboxamide, 10-[4-[([1,1'-biphenyl]-2-ylcarbonyl)amino]-2-chlorobenzoyl]-10,11-dihydro-N-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

L36 ANSWER 9 OF 25 HCA COPYRIGHT 2003 ACS

112:149048 Electrophotographic photoreceptors containing a hydrazone charge-transporting agent. Kuroda, Masami; Nakamura, Yoichi; Kosho, Noboru (Fuji Electric Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 01172967 A2 19890707 Heisei, 7 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1987-332369 19871228.

GI

$$\begin{array}{c|c}
R & \\
N + CH_2 \\
m & S
\end{array}$$

$$\begin{array}{c|c}
CH = CH \\
n & CH = NN
\end{array}$$

$$\begin{array}{c|c}
R^2 \\
R^3 & I
\end{array}$$

AB Electrophotog. photoreceptors exhibiting good sensitivity and cyclicability have a photosensitive layer contg. .gtoreq.1 hydrazones I (R, R1-3 = H, halo, alkyl, alkoxy, acyl, NO2, allyl, aryl; m, n = 0, 1). Thus, an Al-deposited polyester film was coated with a compn. contg. metal-free phthalocyanine, I (R, R1-3 = H; m = 1; n = 0), and Vylon 200 (polyester resin) to give a photoreceptor showing high sensitivity toward both white light and a light of 780 nm.

IT 125863-01-6

RL: USES (Uses)

(charge-transporting agent, for electrophotog. photoconductor, for repeated use)

RN 125863-01-6 HCA

CN 9H-Carbazol-9-amine, N-[[5-(9H-carbazol-9-ylmethyl)-2-thienyl]methylene]-(9CI) (CA INDEX NAME)

L36 ANSWER 10 OF 25 HCA COPYRIGHT 2003 ACS

102:17096 Disposition of nitrofurantoin and nitrofurazone in the isolated perfused rat kidney. Hoener, Betty Ann; Krueger, Terry Ray (Sch. Pharm., Univ. California, San Francisco, CA, 94143, USA). Journal of Pharmaceutical Sciences, 73(11), 1669-71 (English) 1984. CODEN: JPMSAE. ISSN: 0022-3549.

GI

$$O_2N$$
 O
 $CH = NN$
 NH

The disposition of nitrofurantoin (I) [67-20-9] and nitrofurazone [59-87-0] in the isolated rat kidney was detd. The metab. of both nitrofurans could be described by a 1-compartment body model with 1st order elimination kinetics. The total clearances of I and nitrofurazone were not different. However, the fractions excreted unchanged in the urine after 3 h were 0.19 and 0.02, resp., for I and nitrofurazone. Known reduced metabolites of I, the 5-amino deriv. [21997-21-7] and the 5-cyano deriv. [42061-92-7], while not detectable in the perfusate, accounted for .apprx.3% of the dose in the urine. Neither the 5-amino nor the cyano deriv. of nitrofurazone nor the 4-hydroxy deriv. of either compd. was detected. At the conclusion of the 3 h expt., most of the dose of both these nitrofurans was unaccounted for. The perfused kidney appears to metabolize both drugs, although the more toxic nitrofurazone appears to be more extensively metabolized.

IT 42061-92-7

RL: BIOL (Biological study)

(as nitrofurantoin metabolite, in kidney)

RN 42061-92-7 HCA

CN 2-Furancarbonitrile, 5-[[(2,4-dioxo-1-imidazolidinyl)imino]methyl]- (9CI)

(CA INDEX NAME)

L36 ANSWER 11 OF 25 HCA COPYRIGHT 2003 ACS

96:52140 Synthesis of N-(carbonylamino)-1,2,3,6-tetrahydropyridines with analgesic, antiinflammatory, and hyperglycemic activity. Yeung, Jupita M.; Corleto, Linda A.; Knaus, Edward E. (Fac. Pharm. Pharm. Sci., Univ. Alberta, Edmonton, AB, T6G 2N8, Can.). Journal of Medicinal Chemistry, 25(2), 191-5 (English) 1982. CODEN: JMCMAR. ISSN: 0022-2623.

AB A group of N-(carbonylamino)-1,2,3,6-tetrahydropyridines was synthesized to investigate the effects that changes in functionality at the carbonyl group have on analgesic, antiinflammatory, and hyperglycemic activities. One of the most active analgesic compds. was N-[(ethoxycarbonyl)amino]-1,2,3,6-tetrahydropyridine (I), which was 83 times more potent than morphine. Pretreatment with naloxone did not alter the activity of I or of N-[(2-furanylcarbonyl)amino]-1,2,3,6-tetrahydropyridine (II). II was the most potent hyperglycemic agent, elevating blood glucose 181% at 2 and 4 h after 100 mg/kg orally. Several products showed significant antiinflammatory activity.

IT 80431-17-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and analgesic and hyperglycemic activity of)

RN 80431-17-0 HCA

CN 2,6-Pyridinedicarboxamide, N,N'-bis(3,6-dihydro-1(2H)-pyridinyl)- (9CI) (CA INDEX NAME)

L36 ANSWER 12 OF 25 HCA COPYRIGHT 2003 ACS
89:146829 Studies on heterocyclic compounds. XXXV. Synthesis of
furo[3,2-c]pyrazole derivatives. 3. Synthesis of 5-bromomethyl-1,3diphenylfuro[3,2-c]pyrazole and its derivatives. Yoshina, Shigetaka; Kuo,
Sheng-Chu (Fac. Pharm., Meijo Univ., Nagoya, Japan). Yakugaku Zasshi,
98(3), 264-71 (Japanese) 1978. CODEN: YKKZAJ. ISSN: 0031-6903.

Furo[3,2-c]pyrazole derivs. were prepd. to find their biol. activity. Bromination of 5-methyl-1,3-diphenylfuro[3,2-c]pyrazole gave I which was used as the starting material for the synthesis of 1,3-diphenylfuro[3,2-c]pyrazol-5-yl Me ethers, 1,3-diphenylfuro[3,2-c]pyrazol-5-ylmethylamines, 1,3-diphenylfuro[3,2-c-pyrazole-5-acetic acid, and 1,3-diphenylnitrofurylvinylfuro[3,2-c]pyrazole. Satisfactory antibacterial activity in vitro against Staphylococcus, Escherichia coli, Shigella flexneri, Mycobacterium tuberculosis, Candida albicans, and Trichophyton mentagrophytes was found in II (NR1R2 = NHMe, 1-pyrrolidinyl, 4-methyl-1-piperazinyl).

IT 63187-80-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 63187-80-4 HCA

CN 2-Oxazolidinone, 3-[[(1,3-diphenyl-1H-furo[3,2-c]pyrazol-5-yl)methyl]amino]- (9CI) (CA INDEX NAME)

L36 ANSWER 13 OF 25 HCA COPYRIGHT 2003 ACS
89:24214 Studies on heterocyclic compounds. XXXVI. Synthesis of furo[3,2-c]pyrazole derivatives. 4. Synthesis of 1,3-diphenylfuro[3,2-c]pyrazole-5-carboxaldehyde and its derivatives. Yoshina, Shigetaka; Tanaka, Akira; Kuo, Sheng-Chu (Fac. Pharm., Meijo Univ., Nagoya, Japan). Yakugaku Zasshi, 98(3), 272-9 (Japanese) 1978. CODEN: YKKZAJ. ISSN: 0031-6903.

GΙ

AB 1,3-Diphenylfuro[3,2-c]pyrazole-5-carboxaldehyde (I) was prepd. by various methods, and Kroenke's method and oxidn. with tertiary aliph. amine oxide were the most appropriate methods. Reaction of the aldehyde group in I showed that the reactivity of I was similar to that of arom. aldehydes in general, except for benzoin condensation. For example, I gave a

CN

carboxylic acid by oxidn. with Ag2O, an alc. by redn. with NaBH4, and a Schiff base with primary amines. The Cannizzaro reaction, Wittig reaction, and aldol condensation of I gave the anticipated products. Antibacterial tests in vitro of the furo[3,2-c]pyrazoles showed that the condensation product with aminoguanidine had a broad antibacterial spectrum.

IT 63379-36-2P

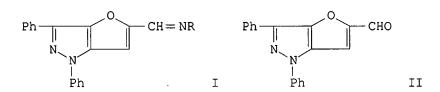
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and bactericidal activity of)

RN 63379-36-2 HCA

2-Oxazolidinone, 3-[[(1,3-diphenyl-1H-furo[3,2-c]pyrazol-5-yl)methylene]amino]- (9CI) (CA INDEX NAME)

L36 ANSWER 14 OF 25 HCA COPYRIGHT 2003 ACS
87:53275 Diphenylfuro[3,2-c]pyrazoles. Yoshina, Shigetaka (Japan). Jpn.
Kokai Tokkyo Koho JP 51125396 19761101 Showa, 3 pp. (Japanese). CODEN:
JKXXAF. APPLICATION: JP 1975-35953 19750325.
GI



The title furopyrazoles I (R = OH, NH2, acylamino, H2NCONH, H2NCSNH, H2NC(:NH)NH, satd. heterocyclyl) were prepd. by reaction of II with RNH2. I had antibacterial, antifungal, and antiprotozoal activity (no data). Thus, aq. soln. of 0.3 g H2NNHCONH2.HCl and 0.36 g AcONa was refluxed 3 h with 1 g II in EtOH to give 1 g I (R = H2NCONH). Among 7 addnl. I similarly prepd. were (R given): OH, H2NC(:NH)NH, H2NCSNH, and MeCONH. IT 63379-36-2P

RN 63379-36-2 HCA

CN 2-Oxazolidinone, 3-[[(1,3-diphenyl-1H-furo[3,2-c]pyrazol-5-yl)methylene]amino]- (9CI) (CA INDEX NAME)

L36 ANSWER 15 OF 25 HCA COPYRIGHT 2003 ACS
87:39474 Furo[3,2-c]pyrazole derivatives. Yoshina, Shigetaka (Japan). Jpn.
Kokai Tokkyo Koho JP 51125298 19761101 Showa, 4 pp. (Japanese). CODEN:
JKXXAF. APPLICATION: JP 1975-35950 19750325.
GI

AB Eighteen furo[3,2-c]pyrazole derivs. I (R1 = lower alkoxy, mono- and dialkylamino, pyrrolidinyl, morpholino, methoxypiperazinyl, etc.) were prepd. by reaction of halomethyl derivs. II (R2 = halo) with R1H. I had antibacterial activity (no data). Thus, 1 g II (R2 = Br) in MeOH was refluxed 2 h to give 83% I (R1 = MeO).

IT 63187-80-4P

RN 63187-80-4 HCA

CN 2-Oxazolidinone, 3-[[(1,3-diphenyl-1H-furo[3,2-c]pyrazol-5-yl)methyl]amino]- (9CI) (CA INDEX NAME)

L36 ANSWER 16 OF 25 HCA COPYRIGHT 2003 ACS
85:77094 Aza-enamines. III. Electrophilic substitution reactions at the azomethine group carbon atom in aldehyde N,N-tetramethylenehydrazones.
Brehme, R.; Nikolajewski, H. E. (Forschungsabteilung, VEB Berlin-Chem., Berlin, Ger. Dem. Rep.). Tetrahedron, 32(6), 731-6 (German) 1976. CODEN: TETRAB. ISSN: 0040-4020.

$$NN = CHR$$
 I $NN = CRCONHSO_2$ $R1$ II

AB The tetramethylenehydrazones I (R = H, Me, Et, CHMe2) with p-R1C6H4SO2NCO (R1 = H, Me) gave the sulfamides II, and I (R = Me, Et) with N-methylenepiperidinium chloride gave the hydrazones III. The results are interpreted in terms of the analogous aza enamine structure of I.

IT 60144-38-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

III

RN 60144-38-9 HCA

CN 1-Pyrrolidinamine, N-[[5-(1-piperidinylmethyl)-2-furanyl]methylene]- (9CI) (CA INDEX NAME)

L36 ANSWER 17 OF 25 HCA COPYRIGHT 2003 ACS
83:206602 Synthesis and investigation of poly(aroylene-s-triazoles). Korshak,
V. V.; Rusanov, A. L.; Leont'eva, S. N.; Dzhashiashivili, T. K. (Inst. Elementoorg. Compd., Moscow, USSR). Macromolecules, 8(5), 582-93
(English) 1975. CODEN: MAMOBX. ISSN: 0024-9297.

GI For diagram(s), see printed CA Issue.

AB Poly(benzoylene-s-triazoles) I (1 isomer shown), poly(isoindolotriazolones) II, and poly(naphthoylene-s-triazoles) III (1 isomer shown), in which Z = m- or p-phenylene, pyridine-2,6-diyl, or bond, and Z1 = 0, S02, or C0, were prepd. by treating bisamidrazones with tetracarboxylic dianhydrides using either multistage polymn. and ring closure or 1-step cyclopolycondensation in polyphosphoric acid. The I were most easily prepd. by the multistage method, and were insol. reddish-black powders which did not soften at 400.degree. and had 5% wt. loss in air at 380-410.degree. The III were prepd. by the 1 state method

and were completely sol: in H2SO4 and MeSO3H, did not soften at 500.degree., and had higher thermal stability than the I due both to higher intrinsic stability of the ring system and higher degree of cyclization. III (Z = m-phenylene) was molded at 350.degree./3500 kg/cm2 into pellets with high ablative stability and fire resistance, with the latter property resulting partially from the presence of residual polyphosphoric acids.

IT 43147-36-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclodehydration of)

RN 43147-36-0 HCA

CN 2,6-Pyridinedicarboximidamide, N,N''-bis(1,3-dioxo-1H-benz[de]isoquinolin-2(3H)-yl)- (9CI) (CA INDEX NAME)

L36 ANSWER 18 OF 25 HCA COPYRIGHT 2003 ACS

83:97125 5-Chloro-2-pyrimidinyl analog of dantrolene. Schwan, Thomas J.; Ellis, K. O. (Norwich Pharm. Co. Div., Morton-Norwich Prod., Inc., Norwich, NY, USA). Journal of Pharmaceutical Sciences, 64(2), 337-8 (English) 1975. CODEN: JPMSAE. ISSN: 0022-3549.

GI For diagram(s), see printed CA Issue.

AB Furamidine-HCl was treated with OHCCCl:CClCO2H and the I (R=H, Rl=CO2H) decarboxylated and formylated to give I (R=CHO, Rl=H), which with 1-aminohydantoin-HCl gave the dantrolene analog II.

IT 56536-55-1P

RN 56536-55-1 HCA

CN 2,4-Imidazolidinedione, 1-[[[5-(5-chloro-2-pyrimidinyl)-2-furanyl]methylene]amino]- (9CI) (CA INDEX NAME)

$$C1 \qquad \qquad CH = N - N \qquad NH$$

L36 ANSWER 19 OF 25 HCA COPYRIGHT 2003 ACS

81:154534 Fluorescent whitening agents for organic polymers. Suzuka,
Masakazu; Matsuo, Masatoshi (Sumitomo Chemical Co., Ltd.). Jpn. Kokai
Tokkyo Koho JP 49053635 19740524 Showa, 4 pp. (Japanese). CODEN: JKXXAF.
APPLICATION: JP 1972-95718 19720922.

AB Compds. of the general formula I (R = alkyl, aralkyl, aryl; R1 = H, alkyl, Ph; X = divalent org. group), prepd. by reaction of N-aminonaphthalimides with XCl2, are fluorescent whiteners for org. polymeric products such as polyacrylonitrile and polyester textiles and polypropylene. For example

fluorescent whitener (II) [53034-60-9] was used to whiten polyacrylonitrile.

IT 53034-60-9

RL: USES (Uses)

(fluorescent brighteners, for acrylic fibers)

RN 53034-60-9 HCA

CN 2,6-Pyridinedicarboxamide, 1,4-dihydro-N,N'-bis(6-methoxy-1,3-dioxo-1H-benz[de]isoquinolin-2(3H)-yl)-4-oxo- (9CI) (CA INDEX NAME)

L36 ANSWER 20 OF 25 HCA COPYRIGHT 2003 ACS

80:47732 Syntheses and antimicrobial activites of 5-cyano-2-furaldehyde and its derivatives. Nakao, Hideo; Fukushima, Masami; Sugawara, Shinichi (Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, Japan). Yakugaku Zasshi, 93(11), 1526-9 (Japanese) 1973. CODEN: YKKZAJ. ISSN: 0031-6903.

AB Reaction of 5-bromo-2-furaldehyde with CuCN gave 5-cyano-2-furaldehyde, which was derivatized via the aldehyde group. No significant antimicrobial activity was found.

IT 42978-22-3P

RN 42978-22-3 HCA

CN 2-Furancarbonitrile, 5-[[(2-oxo-3-oxazolidinyl)imino]methyl]- (9CI) (CA INDEX NAME)

L36 ANSWER 21 OF 25 HCA COPYRIGHT 2003 ACS

79:122194 Potential antimicrobial furans. Hoyle, William; Roberts, Gordon P.; Meth-Cohn, Otto (Pharm. Res. Lab., Ciba-Geigy (UK) Ltd., Manchester, UK). Journal of Medicinal Chemistry, 16(6), 709-10 (English) 1973. CODEN: JMCMAR. ISSN: 0022-2623.

AB Furan derivs. bearing isosteric and isoelec. functional groups in place of a 2-nitro group lacked antibacterial activity, confirming the essential

role of the nitro group in activity. Functional groups employed were sulfo, sulfamoyl, carboxyl, methoxycarbonyl, carbamoyl, and cyano. For example, 5-iodo-2-furaldehyde [2689-65-8] reacted with Cu2(CN)2 in DMF to form 5-formyl-2-furonitrile [42061-89-2], which was condensed with semicarbazide [57-56-7], 3-amino-2-oxazolidinone, or 1-aminohydantoin to yield 5-cyano-2-furancarboxaldehyde semicarbazone [42061-90-5], 3-[(5-cyano-2-furanyl)methylene]amino]-2-oxazolidinone [<math>42061-91-6], and 1-[(5-cyano-2-furanyl)methylene]amino]-2,4-imidazolidinedione (I) [<math>42061-92-7], resp.

IT 42061-92-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and bactericidal activity of)

RN 42061-92-7 HCA

2-Furancarbonitrile, 5-[[(2,4-dioxo-1-imidazolidinyl)imino]methyl]- (9CI) (CA INDEX NAME)

CN

L36 ANSWER 22 OF 25 HCA COPYRIGHT 2003 ACS

79:79242 Benzobis(triazolo)phenanthroline polymers. Evers, Robert C. (Air Force Mater. Lab., Wright-Patterson Air Force Base, OH, USA). Journal of Polymer Science, Polymer Chemistry Edition, 11(7), 1449-63 (English) 1973. CODEN: JPLCAT. ISSN: 0449-296X.

AB Thermally stable benzobistriazolophenanthroline polymers (I, R = 2,6-pyridinediyl, m-phenylene, p-phenylene) were prepd. by condensation of arom. dihydrazidines, e.g. isophthalic dihydrazidine [20439-34-3], with 1,4,5,8-naphthalenetetracarboxylic acid [128-97-2] or its anhydride in polyphosphoric acid, and their structures were detd. by comparison of their spectra with those of prepd. benzotriazolo model compds., e.g. 10-(2-pyridyl)-7H-benzo[de]-s-triazolo[5,1-a]isoquinolin-7-one [41948-45-2]. Degrdn. of I, e.g., poly[(5,8-dihydro-5,8-dioxobenzo[lmn]bis-s-triazolo[5,1-b:1',5'-j][3,8]phenanthroline-2,11-diyl)-2,6-pyridinediyl] [41940-96-9], occurred in air at 440-50.deg., and no softening under load was obsd. at .leq.450.deg..

IT 43147-36-0

RL: USES (Uses) (model compd. for benzobistriazolophenanthroline polymer structure detn.)

RN 43147-36-0 HCA

CN 2,6-Pyridinedicarboximidamide, N,N''-bis(1,3-dioxo-1H-benz[de]isoquinolin-2(3H)-yl)- (9CI) (CA INDEX NAME)

L36 ANSWER 23 OF 25 HCA COPYRIGHT 2003 ACS

69:19623 Poly(pyromellitimideamides). Unishi, Terunobu; Hasegawa, Masak (Fukui Univ., Fukui, Japan). Kogyo Kagaku Zasshi, 70(12), 2392-5 (Japanese) 1967. CODEN: KGKZA7. ISSN: 0368-5462.

GI For diagram(s), see printed CA Issue.

Poly(pyromellitimideamides) were prepd. in 2 steps, i.e., ring-opening polyaddn. and thermal cyclodehydration. When pyromelitic dianhydride was added to aromatic dicarboxylic dihydrazides [R(CONHNH2)2, R = pyridinediyl or C6H4] in a polar solvent, such as HCONMe2, AcNMe2, or Me2SO, polymeric pyromellitic acid dihydrazides of structure I were obtained. The I were sol. in HCONMe2, Me2SO, pyridine, and aq. alkali, and the inherent viscosities varied between 0.3 and 1.7. I (R = 2,6-pyridinediyl) was insol. in AcNMe2, but I (R = 2,5-pyridinediyl or p-C6H4) was sol. Polypyromellitimideamides were synthesized by thermal cyclodehydration of I. The ir spectra of these polymers were compared with those of model compds. D.T.A. and thermogravimetric analyses showed that the cyclocondensation reaction of I was endothermic. The thermal stability of polypyromellitimideamides with R a pyridinediyl group was lower than that of polypyromellitimideamides with R a phenylene group.

IT 32006-70-5P

RN 32006-70-5 HCA

CN Poly[(5,7-dihydro-1,3,5,7-tetraoxobenzo[1,2-c:4,5-c']dipyrrole-2,6(1H,3H)diyl)iminocarbonyl-2,6-pyridinediylcarbonylimino] (8CI) (CA INDEX NAME)

L36 ANSWER 24 OF 25 HCA COPYRIGHT 2003 ACS

62:29608 Original Reference No. 62:5246h Antimicrobials. I. 5-Nitrofuran analogs. Johnston, R. G.; Kidd, David (Pharm. Ind. Ltd., Edinburgh, UK). J. Chem. Soc. (Dec.), 4730-4 (English) 1964.

AB 2-Formyl-6-nitrochromone and -benzothiazole have been synthesized. Their derivs., and new derivs. of 2-formylbenzofuran and -chromone and 7-formyl-3,5-dihydro-4,9- dimethoxy - 2H - furo[3,2 - g]chromen - 5. one, have been screened against gram-pos. and gram-neg. organisms and fungi. .beta.-Vinylogs of 3-(5-nitrofurfurylideneamino)-2-oxazolidinone (furazolidone) have also been examd-

L36 ANSWER 25 OF 25 HCA COPYRIGHT 2003 ACS 62:29607 Original Reference No. 62:5246f-h

62:29607 Original Reference No. 62:5246f-h 6,6-Diphenylnaphtho[1',2':2,3]pyra n and 1,3-diphenyl-3-(1-hydroxy-2-naphthyl)propan-1-one. Cottam, J.; Livingstone, R. (Coll. Technol., Huddersfield, UK). J. Chem. Soc. (Dec.), 5228-31 (English) 1964.

GI For diagram(s), see printed CA Issue.

AB 7,8-Benzocoumarin with phenylmagnesium bromide gives a mixt. contg. 6,6-diphenylnaphtho-[1',2':2,3]pyran and 1,3-diphenyl-3-(1-hydroxy-2-naphthyl)propan-1-one which was easily cyclized and dehydrated to 4,6-diphenylnaphtho[1',2':2,3]pyran (I).

RN 1155-61-9 HCA

CN Pyridinium, 1-[5-[N-(2-oxo-3-oxazolidinyl)formimidoyl]furfuryl]-, chloride (8CI) (CA INDEX NAME)